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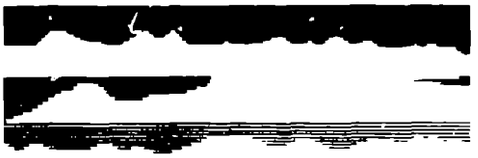

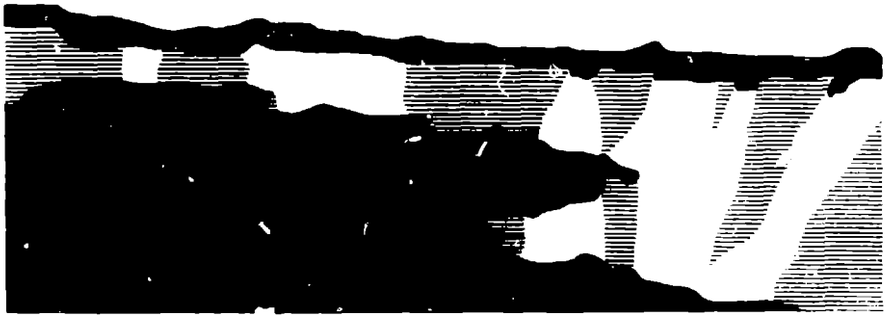

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COUPLED HYDRO-NEUTRONIC CALCULATIONS FOR FAST BURST REACTOR ACCIDENTS

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ABSTRACT

Methods are described for determining the fully coupled neutronic/hydrodynamic response of fast burst reactors (FBR) under disruptive accident conditions. Two code systems, PAD (1-D Lagrangian) and NIKE-PAGOSA (3-D Eulerian) were used to accomplish this. This is in contrast to the typical methodology that computes these responses by either single point kinetics or in a decoupled manner. This methodology is enabled by the use of modern supercomputers (CM-200). Two examples of this capability are presented: an unreflected metal fast burst assembly, and a reflected fast burst assembly typical of the Skua or SPR-III class of fast burst reactor.

I. INTRODUCTION

In the area of fast burst reactors the state-of-the-art allows the production of pulses of a few tens of microseconds with energy yields approaching a few times 10^{17} fissions. FBR accident scenarios with energy releases from 10^{18} to 10^{21} fissions have been postulated in the literature. The physical phenomena range from events which produce small temperature rise to solid-liquid-vapor phase changes through explosive disassembly scenarios. There have been few analytic tools available in the open domain to study this broad range of phenomena.

Historically, there have been several fast burst accidents at the lower end of this range. The early Godiva accident[1] produced approximately 3×10^{17} fissions and rendered the machine inoperable. The fuel was severely oxidized, the bottom center section of the core was thrown across the floor, and there was evidence of fuel melting in the center of the core. The Aberdeen FBR accident[2] produced 6×10^{17} fissions and melted the center of the safety block. Neither of these accidents produced significant explosive effects or any significant release of contamination outside the confinement building.

The safety analysis design basis accidents (DBA) for fast burst reactors[3] includes step reactivity insertions ranging from 0.25 $ to 0.60 $ above prompt critical. The energy release from such accidents range from 10^{18} to 10^{19} fissions. Consequently, a large emphasis is placed on determining the mechanics and processes involved in the most severe accidents. It is the purpose of our research to demonstrate this analysis capability, using modern supercomputers to cost effectively simulate several design basis accidents over a broad range of initial conditions. This paper presents preliminary results of this research.

II. HYDRO-NEUTRONIC CODES

Coupled neutronic-hydrodynamic codes integrate stepwise in space and time the equations describing fission energy generation, energy allocation, and motion. Typically, an excursion code can be thought of as proceeding cyclically from knowledge of the geometry and reactivity to reactor period, power, energy generation, temperatures, pressures, accelerations, velocities, and finally a new geometry and reactivity. This cycle is indicated schematically in Fig. 1.

The variables necessary to describe the system at any given time are postulated to be known, and the procedure necessary to advance the state of the system by one time step are calculated. Now, having completed a time step (or iteration, since both notations are used to describe the cyclic process shown in Fig. 1), all neutronic, thermodynamic, and hydrodynamic variables which characterize the system are updated. The next calculational cycle begins with a quadratic integration of the region volumes and temperatures. Using these volumes and temperatures, the feedback reactivities may be evaluated at time t.

A. One-Dimensional Code: PAD

PAD[4] is a one-dimensional coupled neutronic/hydrodynamic code developed for fast reactor excursions. In

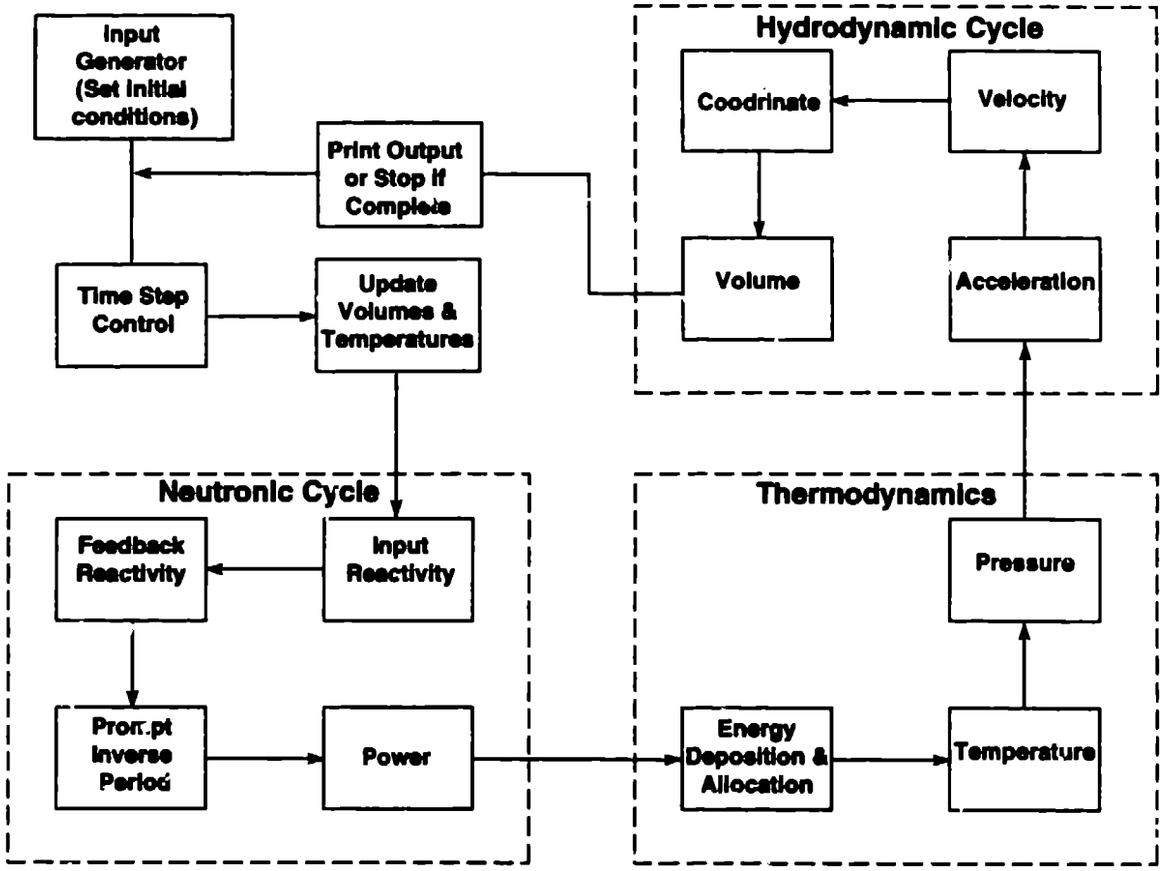

Fig. 1. Schematic diagram of PAD calculational cycle.

spherical geometry, a sphere is divided into concentric shells, known as regions, whose interfaces are located at distances from the center of the system. Contiguous regions with similar neutronic and thermophysical properties may be grouped to form zones. For example, a reactor may consist of a reflected core which contains two fissile element loadings. The PAD model of this system would typically have three zones, one for each core loading and one for the reflector. Each zone would be subdivided into one or more regions.

PAD uses a neutron kinetics formulation with up to six groups of delayed neutrons to describe the time variation of the power in the fissioning system. Throughout a calculation, the spatial power distribution and material motion reactivity feedback are obtained from explicit S_N transport calculations. Differences in the absolute k_{eff} values, or extrapolations thereof, provide the neutronic feedback due to material motion. Temperature feedback effects (Doppler, fuel-pin expansion) are calculated from mathematical models which include spatial reactivity weighting options.

A feature of PAD that has been both useful and often necessary is the decoupling of the neutronic atom densities from the hydrodynamic material densities. An example of the utility of this is the ability to study inertial effects (by varying the material densities) without disturbing the power distribution.

The calculation of fission power density and local energy deposition follows. The energy deposition during the time interval is evaluated and allocated into any of several energy sinks, as dictated by thermodynamic equilibrium and heat transfer conditions: fusion, vaporization, heat transfer, P-dV work, and temperature rise. These five energy sinks may be reversible in PAD. That is, if the thermodynamic conditions are appropriate, a material may solidify, condense, undergo a temperature drop, etc.

After apportioning the internal energy, the pressure is calculated from one, or a combination, of three pressure options: condensed phase (solid and/or liquid), vapor phase, and Van der Waals (liquid and vapor phases). The difference between the pressures of adjacent regions provides the driving force for the calculation of the boundary acceleration, velocity, and position at time t (i.e., the hydrodynamics).

For computing boundary accelerations, the mass associated with a boundary is defined as one-half of the mass of each bounding region. The evaluation of the velocity of the region outer boundary at time t proceeds directly from knowledge of the current acceleration and the previous acceleration and velocity. Similarly, the calculation of the new coordinate, $r(t)$, depends only on its prior value and the current and previous velocities, all of which are known at this time. This completes the calculational cycle shown in Fig. 1 for a region. For this same time and time interval, this cycle is repeated for every region in the system, proceeding spatially outward.

If the volume calculated at the end of the cycle does not match the volume evaluated at the beginning of the cycle (via the open quadratic-integration) to a preset accuracy, then the loop is repeated until the desired convergence has been attained. Additionally, if the calculated temperature or volume of any region is less than zero, or if the region volume changes by more than a prescribed amount relative to the volume at the previous time, the code then provides for automatic time-step reduction. With the reduced time interval, the time cycle, t, is restarted, beginning with the innermost region.

B. Three-Dimensional Code: NIKE/PAGOSA

Three-dimensional calculations were performed using the coupled time-dependent hydrodynamics/neutronics package NIKE/PAGOSA. PAGOSA is a 3-D Eulerian hydrodynamics code[5]; NIKE is a 3-D, multigroup, even-parity neutron transport code. NIKE has options for both discrete ordinates (S_N) and simplified spherical harmonics (SP_N) angular flux treatments.[6] The codes are coupled together intimately through a heat source term determined by NIKE. This term is then used to drive the material motion computed by PAGOSA. The NIKE/PAGOSA flow diagram is shown schematically in Figure 2. The hydrodynamic mesh and material locations are computed by PAGOSA and used by NIKE for neutron transport. NIKE/PAGOSA is written in the new data parallel FORTRAN 90 language and was carefully designed and programmed to run at optimal efficiency on SIMD-like machines such as the Connection Machine CM-200 and CM-5 at Los Alamos National Laboratory (LANL).

PAGOSA is an explicit, 3-D multi-material hydrodynamics code designed to model problems involving high-speed flow and high-rate deformation of solid materials. It has been developed over the past three years on the Connection Machine parallel supercomputer. Finite-difference approximations to the continuum mechanical conservation equations are solved in PAGOSA in an Eulerian frame on a fixed, orthogonal hexahedral grid with

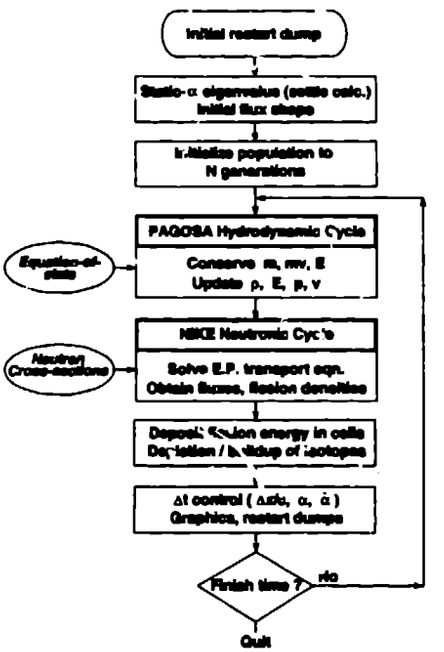

Fig. 2. NIKE/PAGOSA flow diagram.

a Lagrangian/remap algorithm. PAGOSA employs a second-order accurate predictor-corrector method for the Lagrangian phase and a third-order, van Leer-limited upwind scheme for the advection phase. A unique parallel implementation of Young's method for reconstructing interfaces from material volume fraction data enables a Lagrangian-like representation of material interfaces having arbitrarily complex topology.

The NIKE[7,8] code is a implicit time-dependent 3-D multigroup neutron transport code which has been developed over the last two years at LANL for the CM-200. NIKE has two angular discretization options: an discrete-ordinates S_N option and a simplified spherical-harmonic (SP_N) option. Both the S_N and SP_N equations are cast in an even-parity form and solved via a source-iteration technique. The source-iteration equations are solved using a parallel conjugate-gradient method. Both the inner and outer source iterations are accelerated with variants of the diffusion-synthetic technique.[9] These acceleration schemes are sufficiently effective that only one inner iteration per group and one outer iteration per time step are required. Furthermore, they are completely robust and highly effective under all conditions. Either backward-Euler or Crank-Nicholson differencing can be specified for the time variable. NIKE can model both delayed neutrons and fuel depletion. PAGOSA provides NIKE with material and mesh specifications for each time step, and NIKE provides

PAGOSA with energy deposition from neutron reactions in each individual spatial cell.

III. PROBLEM MODELS

For the one-dimensional PAD calculations, each assembly was spherized into a one-dimensional model so as to conserve the total mass of fuel. The fuel for each model was taken to be U(93) metal with a 1. 5% addition of Mo. The Godiva-I critical assembly[10] was modeled as a simple solid sphere of fuel material. The sphere had a radius of 8.8 cm and contained approximately 52.5 kg of fuel.

The Godiva-IV FBR[11] was modeled as a spherical shell with a smaller solid sphere inside the shell separated by a small void shell. The outer shell represents the Godiva-IV fuel rings and control rods, while the inner solid sphere represents the Godiva-IV safety block. The outer fuel shell has an outer radius of 9. 8 cm and an inner radius of 5. 9 cm. The inner solid sphere has a radius of 5. 2 cm. The total mass of fuel for the entire model is approximately 65 kg.

Skua[12] is an annular-core FBR at LANL. The core is an annular cylinder 30.5 cm high with a 24.1-cm inside diameter, a 31.8-cm outside diameter, and a total core mass of 175 kg. It is controlled by means of moveable copper reflectors. The internal core cavity can have a thermalizing "flux trap" present for thermal neutron irradiations. The Skua FBR was modeled as a set of concentric spherical shells surrounding an inner void. The outer shell represents the Skua reflector while the inner shell represents the Skua fuel rings. The fuel shell had an inner radius of 12. 07 cm and an outer radius of 15. 4 cm. The copper reflector shell thickness was 3.4 cm.

A key parameter in the calculation of fast burst dynamics is neutron lifetime. The neutron lifetimes for Godiva-I and Godiva-IV were taken to be 6.0 ns and 6.6 ns, respectively. The neutron lifetime in the burst assembly Skua has been calculated with the flux trap both present and absent. An expression for the system alpha is given by

$$\alpha = \frac{k-1}{\ell},$$

where k is the neutron multiplication factor and ℓ is the neutron lifetime.

Using the discrete ordinates computer code TWODANT,[13] one can calculate both the system alpha and the neutron multiplication factor k. Then using the above expression, the neutron lifetime may be calculated. However, in order to obtain an estimate of the neutron lifetime, one needs accurate estimates of a and k. This requires that the model for TWODANT be extremely refined, i.e., that a large number of mesh points and a high order of S_N be used. To get around these limitations one can do two sets of calculations, the first being the normal system and the second being the system just slightly perturbed. This results in two equations:

$$\alpha_1 = \frac{k_1 - 1}{\ell} \text{ and } \alpha_2 = \frac{k_2 - 1}{\ell}.$$

Since the neutron lifetime is relatively insensitive to small changes in reactivity, we can subtract the two above equations to yield

$$\Delta\alpha = \alpha_1 - \alpha_2 = \frac{k_1 - k_2}{\ell} = \frac{\Delta k}{\ell},$$

and the neutron lifetime may be determined from

$$\ell = \frac{\Delta k}{\Delta \alpha}.$$

The above method for determining the neutron lifetime has been found to be relatively insensitive to the order of S_N and number of mesh points used, as long as the same parameters were used in both calculations. In determining the neutron lifetime for Skua, a detailed physical model was developed which utilized an S_N order of eight with 88 radial and 118 vertical mesh points. Results obtained from TWODANT for Skua near critical indicate that the neutron lifetime with the flux trap is on the order of 47.8 ns and without the flux trap 23.7 ns. To verify this computational technique, as similar calculation was performed on Godiva-IV, which resulted in a calculated neutron lifetime of 5.9 ns, which compares to the measured lifetime of 6.6 ns.

IV. RESULTS

Figure 3 shows the total fission energy yield as a function of initial reactivity step for each critical assembly. The main feature of each curve is the so-called "inertial break," which is the dramatic change in slope of each curve. The inertial breaks occurs between 0.06 and 0.10 $ for the Godiva assemblies and at about 1.0 $ for the Skua assembly. This feature occurs at the onset of inertial effects such as transient mechanical stress and a time lag in fuel material expansion.

Figure 4 show the ratio of kinetic energy to total fission energy as a function of initial reactivity for each assembly. Each curve demonstrates the characteristic behavior of moving asymptotically toward 100% kinetic energy release with increasing reactivity steps.

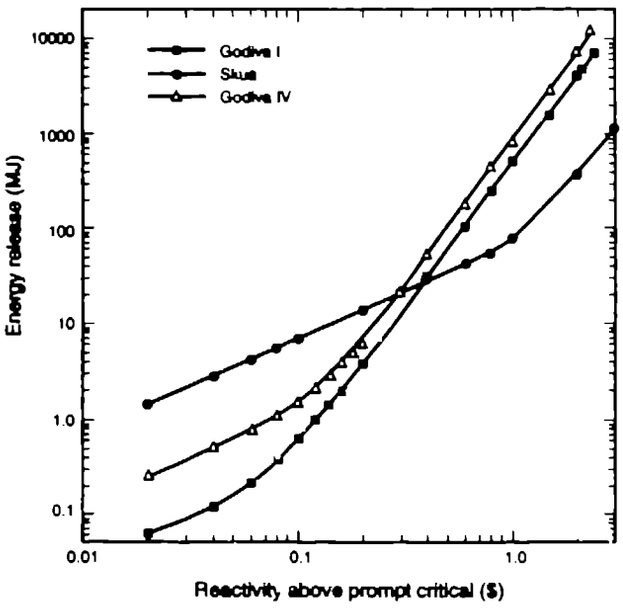

Fig. 3. Total energy release vs initial reactivity step.

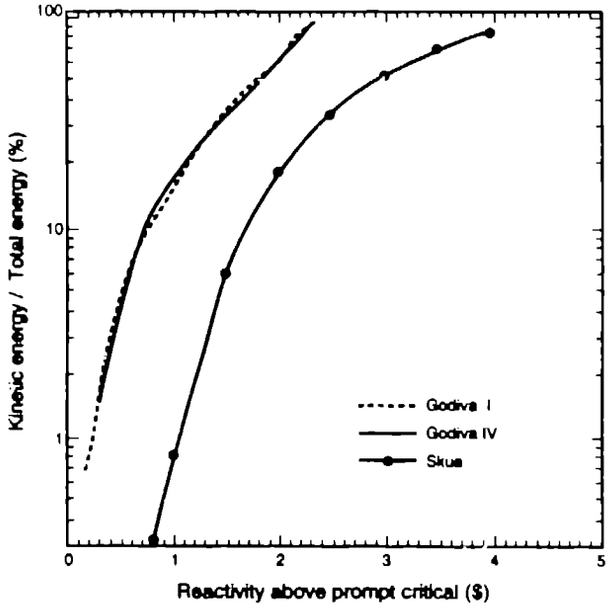

Fig. 4. Ratio of kinetic e .ergy to total energy vs initial reactivity.

These results also illustrate the differences in behavior between the Godiva assemblies and the Skua assembly. The more massive Skua assembly contains more thermal inertia, which produces more yield for the smaller bursts. However, the longer Skua neutron lifetime seems to be delaying the onset of inertial effects for larger bursts.

Initial three-dimensional calculations were performed on a spherical Godiva assembly, from 0.03 $ to several dollars above prompt critical. The step reactivity insertion is added by adjusting the enrichment at $t = 0$. The time-dependent calculation begins with an alpha eigenvalue settle calculation, after which the neutron population is initiated to 15 generations. A comparison of results between NIKE/PAGOSA and the one-dimensional PAD code is shown in Figure 5. The NIKE/PAGOSA runs took from 1.5 to 4.0 hours on the CM-2 using 30x30x30 (27,000 cells) mesh for S_4, 5-group, MENDF/5 (Multi-group ENDF/5) cross sections.

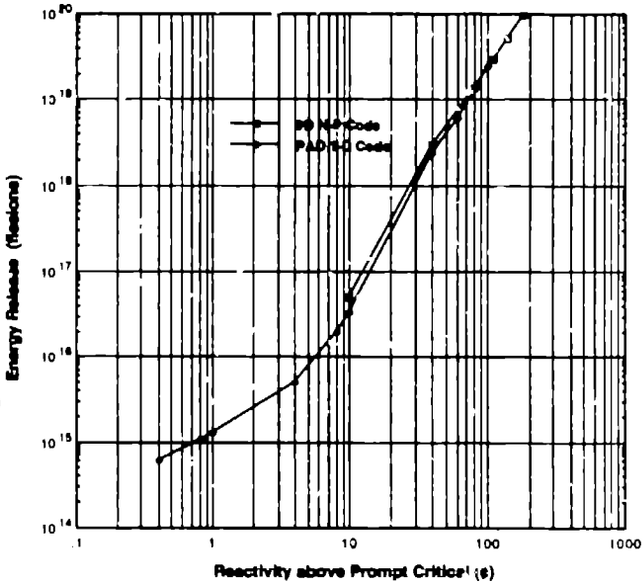

Fig. 5. A comparison between NIKE/PAGOSA and PAD.

V. CONCLUSIONS

In this work we examined hypothetical FBR disruptive accidents with coupled hydro-neutronic codes. We are attempting to extend our research into the use of state-of-the-art three-dimensional codes with modern hydrodynamics and equations-of-state. Results obtained to date have been encouraging, in that two totally distinct code algorithms produce very close results. We are currently examining the sensitivity of energy release to different equations-of-state for U(93)-Mo alloys and several strength-of-materials models. We envision the possibility of calculating realistic 3-D models of all current burst reactors (Godiva-IV, Skua, SPR-II and SPR-III, the WSMR Molly-G, and the APRF Fast Burst Reactor). In addition, we hope to examine a number of postulated criticality and auto-catalytic accidents, and events such as Kiwi-TNT and Chernobyl.

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